



chain nodes :

9 10 11 12 13 17 18 21 22

ring nodes :

1 2 3 4 5 6 7 8 14

chain bonds :

7-9 8-13 9-10 9-17 9-18 10-11 10-12 11-21 11-22

ring bonds :

1-3 1-2 2-5 3-4 4-6 5-6 5-7 6-14 7-8 8-14

exact/norm bonds :

5-7 6-14 7-8 7-9 8-13 8-14 9-10 9-17 9-18 10-11 10-12 11-21 11-22

normalized bonds :

1-3 1-2 2-5 3-4 4-6 5-6

G1:C,O,S,N

G2:H,X,Cb,Cy,Hy,Ak

G3:H,Cb,Cy,Hy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:Atom 17:CLASS 18:CLASS 21:CLASS 22:CLASS